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Abstract: In this work, we propose a numerical method for the modelling of phase transitions in compressible fluid flows. The pressure laws taking into account phase transitions are complex and lead to difficulties such as the non-uniqueness of the entropy solutions. In order to avoid these difficulties, we propose a projection finite volume scheme. It is based on a Riemann solver with a simpler pressure law and an entropy maximization procedure in order to recover the original complex pressure law. Several numerical experiments are presented which validate this approach.

Key-words: Cavitation, Godunov scheme, Two-phase compressible flow.

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Simulation par volumes finis d'écoulements cavitants

Résumé : Nous proposons une méthode numérique pour la modélisation des transitions de phase dans un écoulement compressible. Les lois de pression permettant de modéliser les transitions de phase sont en général complexes et conduisent à des difficultés telles que la non unicité des solutions entropiques. Pour résoudre ce problème, nous proposons un schéma de volumes finis relaxé. Ce schéma est basé sur un solveur de Riemann pour une loi de pression plus simple. Une procédure d'optimisation de l'entropie de mélange à chaque pas de temps permet de revenir à la loi de pression complexe. Plusieurs résultats numériques viennent valider notre approche. En particulier, le schéma permet de sélectionner l'unique solution physique.

Mots-clés : Cavitation, schéma de Godunov, écoulements diphasiques compressibles.

1. Introduction

This work is devoted to the numerical modelling of phase transition in compressible fluid flows. We focus on the liquid-vapor phase transition also called *cavitation*. For this we consider the Euler system for an inviscid and compressible fluid (2.1) together with a pressure law (2.2) which insures the hyperbolicity of the Euler system. This system has been extensively studied, both theoretically and numerically. Standard textbooks exist now on this subject [11], [22], [23]. The existence and uniqueness of a solution to this system, for a general initial condition, is still an open question.

On the other hand, the Riemann problem, which consists to find in one dimension a solution for a particular initial condition made of two constant states, is perfectly understood. It is known that a supplementary dissipation criterion must be added in order to recover uniqueness. This criterion can have several forms. The most classical criterions are:

(1) The Lax entropy criterion: it expresses that any Lax entropy should increase in shocks.
(2) The Lax characteristic criterion: it expresses that a shock of the $i-$th family should be crossed by the $i-$th characteristics coming from the two sides of the shock.
(3) The vanishing viscosity criterion: it expresses that the solution should be the limit of solutions of the Euler system perturbed by a supplementary viscosity term.

In the case of a simple pressure law, such as the perfect gas, it appears that these three criterions are equivalent. But for more complex laws used for the modelling of phase transitions, the good criterion is the viscosity criterion. In some configurations, one can indeed find several solutions satisfying criterion 1 or 2, even if the pressure law insures the hyperbolicity of the system. More precisely, the previous criterions are ordered from the weakest to the strongest. A very detailed study of these topics can be found in the thesis of Jaouen [13]. In this reference a proof of non-uniqueness is also given in the case of a simplified phase transition pressure law.

For classical pressure laws, the Riemann problem solution is made of several constant states separated by shock waves, simple waves and a contact discontinuity. Phase transition pressure laws may present pathologies such as slope discontinuities, lack of convexity of the isentropes or of the Hugoniot curves in the (τ, p) plane... These pathologies lead to a more complex resolution of the Riemann problem. One has to take into account the possibility of composite waves. This subject is studied in the paper of Menikoff and Plohr [17]. Classical references about the Riemann problem for arbitrary fluids are also [5], [25], [24]. Thus, even if the Riemann problem is still uniquely solvable, it is difficult to practically implement it in a Godunov type scheme.

Several numerical methods have been proposed to solve the Euler system with complex pressure laws. Some methods rely on approximate Riemann solvers [10], [13], [2]. These methods must be carefully employed because even if the scheme is entropic it may converge

towards wrong solutions due to the non-uniqueness of the solution. This possible behavior is illustrated in [13], where an entropic Godunov type scheme converges to different solutions according to the CFL number.

In this paper we focus on special pressure laws. We suppose that the pressure law is obtained from a physical entropy maximization with respect to hidden variables. This is not a restriction for phase transitions because it is exactly the way the liquid-vapor mixture is classically modelled [6]. We then use this representation in order to design a finite volume scheme (which we first described in [12] and [3]). Each time-step of this scheme is made of two sub-steps:

(1) A standard Godunov resolution taking into account the hidden variables. In this step, the hidden variables are simply convected with the fluid. It appears that the associated Riemann problem is easier to solve than the original one. Indeed, the relaxed pressure law with hidden variables has no pathology. This step is entropic because we use an exact Riemann solver.
(2) Then, the conservative variables are kept for the next time step. The pressure is actualized by maximizing the physical entropy with respect to the hidden variables. This amounts to project the relaxed pressure law towards the real pressure law. This step is also entropic by construction.

The paper is thus organized as follow.

Following this Introduction, the second part is devoted to a presentation of a simple mathematical framework for the modelling of phase transition. We consider the flow of a compressible liquid which is subject to phase transition (vaporization). The idea is to add to the initial Euler system (2.1) a convection equation with a relaxation source term (see (2.13) and (2.16)) for a supplementary vector $Y(t,x)$ called the fractions vector (which plays the role of the hidden variables). The complex initial pressure law is replaced by a simpler pressure law (2.5) which depends on density, internal energy and the fractions. To this simpler pressure law is associated an entropy. We then define the equilibrium fractions Y_{eq} of the relaxation source term (2.16) by an optimization of the entropy with respect to Y. We suppose that the complex pressure law is recovered by replacing Y with Y_{eq} in the simple pressure law.

The idea to replace a complex pressure law by a simpler one together with a relaxation procedure has been first proposed by Coquel and Perthame in [8]. This idea has also been exploited in [7], [15] for the modelling of two-phase flows without phase transition. Even when the two phases are supposed to be non-miscible, it is necessary, for numerical reasons, to define a mixture pressure law. This mixture pressure law is obtained by imposing pressure equilibrium between the two phases. It appears to be quite complicated. Thus, in order to use an exact Riemann solver, it is interesting to relax the pressure law. This is done in [7], [15] by solving a supplementary convection equation for the volume fraction of one fluid. At the end of each time step, this volume fraction is modified in order to recover the pressure

equilibrium.

We then apply the previous mathematical framework to a physical model of vapor-liquid mixture. We first recall some well known facts about thermodynamics of mixtures. We consider two fluids which are supposed to be non miscible at a small scale. The behavior of each fluid is entirely described by its specific entropy which is a function of the specific volume $\tau = 1/\rho$, where ρ is the density, and of the internal energy ε. The caloric law is recovered with the derivative of the entropy with respect to ε. The pressure law is obtained with the derivative of the entropy with respect to τ. Some classical notions are recalled: volume fraction α, mass fraction y and energy fractions z of the vapor in the mixture. We are then led to define the fraction vector $Y = (\alpha, y, z)^T$ whose each component is between 0 and 1. Using the physical fact that the entropy is an extensive variable, it is then possible to get in a unique manner the mixture entropy s, function of the specific volume, the internal energy and of the fractions $Y = (\alpha, y, z)^T$. Then, the second principle of thermodynamics tells us that the equilibrium fractions must realize a maximum of the mixture entropy. An important fact is that this maximum is under the constrain that all components of Y are between 0 and 1. Thus it does not necessarily imply that the gradient of s with respect to Y is zero. If the maximum is attained in the interior of the constrain set, we recover the fact that an equilibrium is possible when the pressures, temperatures and chemical potentials of the two phases are identical (see (2.27), (2.28), (2.29)). On the other hand, the maximum can be attained on the boundary of the constrain set. In this case, only one phase is stable.

In the third part of the paper, we applied the previous theory to a mixture of two phases satisfying the stiffened gas equation of state (3.1). In order to have simpler computations, we suppose that the thermal equilibrium always holds. In this way, it is possible to eliminate the energy fraction from the unknowns. Then, an important feature is that the resulting mixture pressure law is still a stiffened gas law. But the equilibrium pressure law is no more a stiffened gas law.

Then we again simplify the model by supposing that the two phases are perfect gases. In this case, it is also possible to eliminate the volume fraction in the model, the only remaining fraction is then the mass fraction y. The mixture pressure law is still a perfect gas law. If one optimizes the mixture entropy with respect to y we recover the phase transition model studied by Jaouen in [13].

The fourth part is devoted to the study of the Riemann problem associated to the pressure law of the previous section. We briefly explain how it is possible to construct several entropy solutions to the Riemann problem. This construction is not original and is entirely contained in the thesis of Jaouen [13]. First, an entropy shock solution is constructed. The right state of the shock is in a pure phase while the left state lies in the saturation region (the two phases are at equilibrium). Another solution is also constructed with the same right and left initial states. It is composed of 3 shocks and a contact discontinuity. It is proved in [13] that this latter solution is the only one which possesses a viscous profile. It is

thus the good "physical" solution.

In the fifth part, we present the projection scheme and validate it on the analytical solution build in section four. The description is very simple. Each time step of the finite volume scheme is made of two stages. In the first stage, a simple Godunov scheme is employed. Thus, the source term in the fractions convection equation (2.13) is not taken into account. Because in this stage the pressure law is simplified, it is possible to use an exact Riemann solver and to have the correct entropy dissipation. In the second stage, the fraction vector Y is modified in such a way to maximize the entropy of the mixture in each cell. This stage is conservative, because the density, velocity and energy are not modified. It is also entropy dissipative by construction.

We illustrate then the projection scheme on the very simple test case of a double rarefaction wave in a water flow. If the phase transition were not taken into account, we would observe that the density of water, even in the rarefaction region, would remain of the order of 1000kg.m^{-3} and that the pressure would become strongly negative. Indeed, negative pressures can locally and briefly appear in a liquid, they should then be called *tensions*. But in the zone of negative pressures the liquid would then be in a metastable state and would be subject to vaporization. It must be pointed out that if the cavitation is not taken into account, the apparition of negative pressures is neither a mathematical nor a numerical problem. For example, the model is still hyperbolic. For more details on this subject, we refer to our previous works [4]. If the entropy is optimized with respect to Y at each time step we observe then the apparition of a vapor bubble in the middle of the computation domain. The density in the bubble is much lower and the pressure remains positive. The qualitative behavior of the projection scheme is thus satisfying. We also verify quantitatively that it is able to reproduce the physical entropy solution constructed in section four. It is important to notice here that the numerical solution does not depend on the CFL number. We explain the good behavior of the projection scheme by the fact that the production of entropy occurs not only in the Godunov step but also because of the phase transition. It is important because a global entropy production is not sufficient. One could imagine, for example, a non-physical shock in the metastable model, with a local decrease of entropy, compensated by the entropy production due to the phase transition. The global entropy production can be positive, but the solution is not physical.

Section 6 is then devoted to a 2D simulation in order to illustrate the ability of our scheme to deal with physical configurations. This test is very similar to the one proposed by Butler, Cocchi and Saurel in [21]. The goal is to compute the flow around an hypersonic projectile dived into water at a velocity of 1000 m/s. A strong depression appears in the wake of the projectile, triggering the growth of a cavitation pocket. We are able to reproduce correctly this phenomenon.

The paper ends with a conclusion (part 7).

2. Mathematical models for phase transition

We consider the two-phase vapor-liquid mixture as a single compressible medium with (in 1D) density $\rho(t,x)$, velocity $u(t,x)$, internal energy $\varepsilon(t,x)$ and pressure $p(t,x)$, all depending on the time variable t and the space variable x. Conservation of mass, momentum and energy and Newton's law for inviscid flow lead to the three Euler equations:

$$\begin{aligned} \rho_t + (\rho u)_x &= 0, \\ (\rho u)_t + (\rho u^2 + p)_x &= 0, \\ (\rho\varepsilon + \rho u^2/2)_t + ((\rho\varepsilon + \rho u^2/2 + p)u)_x &= 0. \end{aligned} \tag{2.1}$$

If the flow is not too fast, i.e. if the equilibrium between the liquid and its vapor is achieved for all (t,x), the pressure of the whole mixture depends only on the density ρ and the internal energy ε. We shall write

$$p = p_{eq}(\rho, \varepsilon). \tag{2.2}$$

This equilibrium pressure law is generally quite complex, and more important, leads to unclassical behaviors of the solutions: non-uniqueness of the entropy solution, composite waves. We insist on the fact that it has nothing to do with a defect of hyperbolicity. Phase transition pressure laws naturally insures the hyperbolicity. For example, the Van der Waals pressure law is a bad model of phase transition. It has to be modified by the Maxwell's construction in order to eliminate the elliptic region, and the modified law insures hyperbolicity.

We propose in this section a more general model, in which we do not suppose anymore the equilibrium of the two-phase mixture. We have thus to introduce supplementary variables and the pressure will also depend on these variables. This pressure law will be called the relaxed pressure law. Because the resulting model is out of equilibrium, we shall denote it as the metastable model.

Of course we will also have to go back to the equilibrium pressure law. This will be done thanks to a projection method. Although it would be interesting to account for the dynamic of the phase transition, we do not deal with this problem here and just use the metastable model in order to compute the equilibrium model.

2.1. **A generalized metastable model.**

A supplementary vector of variables, called the *fractions vector* $Y(t,x)$ is used in order to model vaporization. The components Y^i, $1 \leq i \leq p$ satisfy

$$0 \leq Y^i \leq 1. \tag{2.3}$$

We also suppose that when the fluid is pure liquid $Y^i = 0$, and when the fluid is pure vapor $Y^i = 1$. When no phase transition occurs, there is no transfer between the liquid and its vapor, thus we also have perfect convection of the fractions:

$$Y_t + uY_x = 0. \tag{2.4}$$

We have to close these equations with a pressure law

$$p = p(\rho, \varepsilon, Y). \tag{2.5}$$

When equations (2.1), (2.4) and (2.5) are considered, we will speak of the *metastable model*. Indeed, in this model the fraction are simply convected in the flow, and thus, there is no transfer between the two phases.

It is well known that the solution of model (2.1), (2.4), (2.5) is not unique and that a supplementary condition has to be added to restrict the set of solutions. For a simple pressure law, this can be an entropy growth criterion. But it can be necessary to envisage other criterions as described in the Introduction. With $\tau = 1/\rho$, an entropy is a concave function $s = s(\tau, \varepsilon, Y)$ solution of the first order PDE

$$s_\tau - p(1/\tau, \varepsilon, Y) s_\varepsilon = 0. \tag{2.6}$$

Generally, one can find several entropies. Defining the temperature by

$$T = 1/s_\varepsilon, \tag{2.7}$$

we recover the classical relation

$$T ds = d\varepsilon + p d\tau. \tag{2.8}$$

Thus, choosing an entropy amounts to choose the temperature scale. It permits also to recover the pressure law by

$$p = T s_\tau. \tag{2.9}$$

A given entropy is called a *complete equation of state* (see [17]) because it permits to recover the pressure law (2.9) and the caloric law (2.7). When one studies the dynamic behavior of a compressible fluid, an incomplete equation of state (the pressure law) is sufficient. But if one wishes to model a thermodynamic feature such as the phase transition, it is necessary to fix the temperature scale and thus a complete equation of state is required. In the sequel, we then suppose that one particular entropy has been selected. The construction of the mixture entropy from the entropies of the two phases and from physical considerations is described below.

Simple computations shows that a regular solution of system (2.1), (2.4), (2.5) satisfies

$$s_t + u s_x = 0, \tag{2.10}$$

which can be cast into a conservative form

$$(\rho s)_t + (\rho u s)_x = 0. \tag{2.11}$$

When dealing with discontinuous solutions, the latter has to be replaced by an inequation in order to recover uniqueness

$$(\rho s)_t + (\rho u s)_x \geq 0. \tag{2.12}$$

2.2. **Entropy compatible transition models.** In order to take phase transition into account, we have to add a source term to equation (2.4)

$$Y_t + uY_x = \mu. \tag{2.13}$$

Equations (2.1), (2.5) together with (2.13) will be referred as the cavitation or *transition model*. In the case where the phase transition is infinitely fast, we will always have

$$Y = Y_{\text{eq}}(\rho, \varepsilon), \tag{2.14}$$

because the repartition of liquid and vapor is completely determined by the phase diagram. We require that the resulting pressure law is exactly the equilibrium pressure law (2.2)

$$p = p(\rho, \varepsilon, Y_{\text{eq}}(\rho, \varepsilon)) = p_{eq}(\rho, \varepsilon). \tag{2.15}$$

It is then natural to consider (as in [8]) a relaxation source term of the form

$$\mu = \lambda(Y_{\text{eq}}(\rho, \varepsilon) - Y), \tag{2.16}$$

and letting $\lambda \to \infty$.

Suppose then that the equilibrium fractions Y_{eq} are defined by

$$s(\rho, \varepsilon, Y_{\text{eq}}(\rho, \varepsilon)) = \max_{Y \in Q} s(\rho, \varepsilon, Y), \tag{2.17}$$

where Q is the set of admissible parameters. Then, thanks to the concavity of s, for the cavitation model we have also

$$\begin{aligned} s_t + us_x &= \nabla_Y s \cdot (Y_t + uY_x)\,, \\ &= \lambda \nabla_Y s \cdot (Y_{\text{eq}} - Y) \\ &\geq \lambda\,(s(Y_{\text{eq}}) - s(Y)) \\ &\geq 0, \end{aligned} \tag{2.18}$$

The entropy condition is thus reinforced when compared to the metastable model because the production of entropy occurs not only in shocks but also because of the phase transition. It is important because a global entropy production is not sufficient. One could imagine, for example, a non-physical shock in the metastable model, with a local decrease of entropy, compensated by the entropy production due to the phase transition. The global entropy production can be positive, but the solution is not physical (see [13] and section (4.2)).

2.3. **Mixture entropy.** The mathematical framework is now set. We show in this section that it is possible to construct a physical model for phase transition flows inside this framework. We have first to consider the thermodynamic behavior of a mixture of two fluids.

Let V be a small volume occupied by the two fluids which we index by (1) and (2). The fluid (i) fills a volume V_i in V and we have $V_1 + V_2 = V$, i.e. the two fluids are not miscible at a small scale. The volume fraction of fluid (i) is defined by

$$\alpha_i = \frac{V_i}{V}. \tag{2.19}$$

At a small scale, the density of fluid (i) is $\overline{\rho}_i$. But because fluid (i) does not fill all the volume V, the apparent density (at large scale) is $\rho_i = \alpha_i \overline{\rho}_i$. The mixture density is $\rho = \rho_1 + \rho_2$. The mass fraction of fluid (i) is defined by

$$y_i = \frac{\rho_i}{\rho}. \tag{2.20}$$

On the other hand, the large scale massic energy is linked to the small scale massic energy by $\varepsilon_i = y\overline{\varepsilon}_i$. It is then possible to define the energy fraction of fluid (i) by

$$z_i = \frac{\varepsilon_i}{\varepsilon}. \tag{2.21}$$

We also set $\alpha = \alpha_1$, $y = y_1$, $z = z_1$ (and thus $\alpha_2 = 1 - \alpha$, $y_2 = 1 - y$, $z_2 = 1 - z$).

Now, the thermodynamic behavior of each fluid is completely determined by its specific (i.e. per mass unity) entropy function

$$s_i = s_i(\overline{\tau}_i, \overline{\varepsilon}_i), \tag{2.22}$$

where we have defined the specific volume τ by $\tau = 1/\rho$. Indeed, as already explained before, the caloric law, which expresses the temperature T_i of fluid (i), is recovered by

$$\frac{1}{T_i} = \frac{\partial s_i}{\partial \overline{\varepsilon}_i}, \tag{2.23}$$

and the pressure law is given by

$$\frac{p_i}{T_i} = \frac{\partial s_i}{\partial \overline{\tau}_i}. \tag{2.24}$$

Then according to the second principle of thermodynamics, the entropy is an extensive variable. Setting $Y = (\alpha, y, z)^T$, it means that the mixture specific entropy is necessarily given by

$$s(\tau, \varepsilon, Y) = y s_1(\frac{\alpha}{y}\tau, \frac{z}{y}\varepsilon) + (1-y) s_2(\frac{1-\alpha}{1-y}\tau, \frac{1-z}{1-y}\varepsilon). \tag{2.25}$$

It is easy to check that s is concave with respect to (τ, ε, Y), thanks to the concavity of s_i.

According to the second principle, we also know that the equilibrium fractions vector must satisfy

$$s(\tau, \varepsilon, Y_{\text{eq}}) = \max_{0 \le Y \le 1} s(\tau, \varepsilon, Y). \tag{2.26}$$

When the maximum is attained in the interior of the constrain set, i.e. if $0 < Y_{\text{eq}} < 1$, it is characterized by

$$\frac{\partial s}{\partial \alpha} = \tau(p_1 - p_2) = 0, \tag{2.27}$$

$$\frac{\partial s}{\partial z} = \varepsilon(T_1 - T_2) = 0, \tag{2.28}$$

$$\frac{\partial s}{\partial y} = -(\mu_1/T_1 - \mu_2/T_2) = 0, \tag{2.29}$$

where μ_i is the specific Gibbs function of fluid (i) (or the fluid (i) chemical potential) defined by

$$\mu = \varepsilon + p\tau - Ts. \tag{2.30}$$

We recover the well known fact that a phase transition occurs at constant temperature and pressure and that on the saturation curve, the chemical potentials are equal.

The mixture entropy (2.25) also defines a mixture pressure law and a caloric law:

$$p = Ts_\tau = T(\alpha p_1/T_1 + (1-\alpha)p_2/T_2), \tag{2.31}$$

$$\frac{1}{T} = \frac{z}{T_1} + \frac{1-z}{T_2}. \tag{2.32}$$

3. A simple pressure law for phase transition

3.1. **Mixtures of stiffened gases.** We now consider here a simple case where the entropies of the two fluids are

$$s_i = C_i \ln((\overline{\varepsilon}_i - Q_i - \pi_i\overline{\tau}_i)\overline{\tau}_i^{\gamma_i - 1}) + s_i^0. \tag{3.1}$$

Thus, the caloric law and the pressure law are those of a stiffened gas

$$\begin{aligned} C_iT_i &= \overline{\varepsilon}_i - Q_i - \pi_i\overline{\tau}_i, \\ p_i &= (\gamma_i - 1)\overline{\rho}_i(\overline{\varepsilon}_i - Q_i) - \gamma_i\pi_i. \end{aligned} \tag{3.2}$$

We also have

$$p_i + \pi_i = (\gamma_i - 1)\overline{\rho}_i C_i T_i. \tag{3.3}$$

A further simplification will be to suppose the temperature equilibrium, $T = T_1 = T_2$. The variable z can then be eliminated. Setting

$$C = yC_1 + (1-y)C_2, \tag{3.4}$$

$$Q = yQ_1 + (1-y)Q_2, \tag{3.5}$$

$$\pi = \alpha\pi_1 + (1-\alpha)\pi_2, \tag{3.6}$$

$$\gamma = \frac{y\gamma_1 C_1 + (1-y)\gamma_2 C_2}{yC_1 + (1-y)C_2}, \tag{3.7}$$

we obtain

$$p = (\gamma - 1)\rho CT - \pi, \tag{3.8}$$

$$CT = \varepsilon - Q - \frac{\pi}{\rho}. \tag{3.9}$$

In this way, the mixture behaves as a stiffened gas. It must be noted that the elimination of the energy fraction z is necessary in order that the mixture behaves like a stiffened gas. On the other hand, if one eliminates also the volume fraction α by imposing the pressure equilibrium, then the pressure law is no more a stiffened gas law (except when the two phases satisfy $\pi_i = 0$, i.e. when they are perfect gases). The interest of the stiffened gas law is that

the associated Riemann problem is easy to solve exactly and this fact will be exploited in the numerical method below.

The entropy of the mixture is

$$
\begin{aligned}
&s(\tau,\varepsilon,\alpha,y) = C\ln(\varepsilon - Q - \pi\tau) - C\ln C + (\gamma-1)\ln\tau \\
&+\ln\left(\left(\frac{\alpha}{y}\right)^{yC_1(\gamma_1-1)}\left(\frac{1-\alpha}{1-y}\right)^{(1-y)C_2(\gamma_2-1)}\right) + Ky.
\end{aligned}
\tag{3.10}
$$

3.2. **Mixtures of perfect gases.** In this section, we consider the simplest case of a mixture of perfect gases at constant pressure and temperature, thus the entropies are given by (we have set $\Gamma = \gamma - 1$)

$$
s_i = \ln((\overline{\varepsilon}_i\overline{\tau}_i)\overline{\tau}_i^{\Gamma_i}).
\tag{3.11}
$$

The equilibrium of temperature is expressed by

$$
T_1 = T_2 \Rightarrow \varepsilon = y\overline{\varepsilon}_1 + (1-y)\overline{\varepsilon}_2 = yT_1 + (1-y)T_2 = T.
\tag{3.12}
$$

And then, the equilibrium of pressures gives

$$
\begin{aligned}
&p_1 = \Gamma_1\overline{\varepsilon}_1/\overline{\tau}_1 = p_2 = \Gamma_2\overline{\varepsilon}_2/\overline{\tau}_2, \\
&\Gamma_1\frac{y}{\alpha} = \Gamma_2\frac{1-y}{1-\alpha}.
\end{aligned}
\tag{3.13}
$$

We can thus express α in function of y.

$$
\alpha = \frac{\Gamma_1 y}{\Gamma}, \quad 1-\alpha = \frac{\Gamma_2(1-y)}{\Gamma}, \quad \text{with} \quad \Gamma = y\Gamma_1 + (1-y)\Gamma_2.
\tag{3.14}
$$

Finally, the mixture entropy is

$$
\begin{aligned}
&s = y\ln\left(\varepsilon\left(\frac{\Gamma_1}{\Gamma}\tau\right)^{\Gamma_1}\right) + (1-y)\ln\left(\varepsilon\left(\frac{\Gamma_2}{\Gamma}\tau\right)^{\Gamma_2}\right), \\
&= \ln\varepsilon + \Gamma\ln\tau + y\Gamma_1\ln\Gamma_1 + (1-y)\Gamma_2\ln\Gamma_2 - \Gamma\ln\Gamma.
\end{aligned}
\tag{3.15}
$$

The fraction vector Y is in this case reduced to the mass fraction y. But the mixture is still a perfect gas.

In the sequel, we suppose that $\Gamma_1 > \Gamma_2$ (i.e. the phase (1) is less dense than the phase (2)). The derivative of s with respect to y is

$$
\begin{aligned}
&\frac{\partial s}{\partial y} = (\Gamma_1-\Gamma_2)\ln\tau + \Gamma_1\ln\Gamma_1 - \Gamma_2\ln\Gamma_2 \\
&-(\Gamma_1-\Gamma_2)\ln\Gamma - (\Gamma_1-\Gamma_2).
\end{aligned}
\tag{3.16}
$$

The saturation curve for this phase transition model is defined by $\frac{\partial s}{\partial y} = 0$. We find that the saturation curve is in the plane (T, p) a straight line of equation

$$\frac{T}{p} = \exp(1) \ln \left(\frac{\Gamma_2^{\Gamma_2}}{\Gamma_1^{\Gamma_1}} \right)^{\frac{1}{\Gamma_1 - \Gamma_2}} = G. \tag{3.17}$$

Maximizing s with respect to y under the constraints $0 \leq y \leq 1$ permits to recover the equilibrium pressure law

$$\begin{cases} p_{eq}(\tau, \varepsilon) = \Gamma_2 \varepsilon / \tau & \text{if } \tau \leq \tau_2, \\ p_{eq}(\tau, \varepsilon) = G\varepsilon & \text{if } \tau_2 \leq \tau \leq \tau_1, \\ p_{eq}(\tau, \varepsilon) = \Gamma_1 \varepsilon / \tau & \text{if } \tau \geq \tau_1, \end{cases} \tag{3.18}$$

with

$$\tau_i = G\Gamma_i. \tag{3.19}$$

This model is exactly the one proposed by Jaouen in [13].

4. Construction of an analytical solution

In this part, we consider the Euler system (2.1) and the pressure law (3.18). The Euler system can also be written

$$W_t + F(W)_t = 0, \tag{4.1}$$

with $W = (\rho, \rho u, \rho\varepsilon + \rho u^2/2)^T$. We will also use a privileged set of non-conservative variables that we note $V = (\tau, u, p)^T$. We recall briefly how it is possible to construct several entropy solutions to the Riemann problem, which consists to find solutions to (2.1) when the initial condition is

$$W(0, x) = \begin{cases} W_l & \text{if } x < 0, \\ W_r & \text{if } x > 0. \end{cases} \tag{4.2}$$

We will compute precisely the correct entropy solution, which is the limit of viscosity solutions. This analytical solution will be used to validate our scheme in section 5.3.

4.1. **A simple entropy shock solution.**

We will only consider solutions made of one or several shock waves. A shock solution of velocity σ has the form

$$W(0, x) = \begin{cases} W_l & \text{if } x/t < \sigma, \\ W_r & \text{if } x/t > \sigma. \end{cases} \tag{4.3}$$

The Rankine-Hugoniot shock condition must be satisfied. Denoting $[\phi]$ the jump of the quantity ϕ across the discontinuity ($[\phi] = \phi_r - \phi_l$), they can be written $\sigma[W] = [F(W)]$ or

$$\begin{aligned} &\sigma \left[\rho\right] = \left[\rho u\right], \\ &\sigma \left[\rho u\right] = \left[\rho u^2 + p\right], \\ &\sigma \left[\rho\varepsilon + \rho\frac{u^2}{2}\right] = \left[\left(\rho\varepsilon + \rho\frac{u^2}{2} + p\right) u\right]. \end{aligned} \tag{4.4}$$

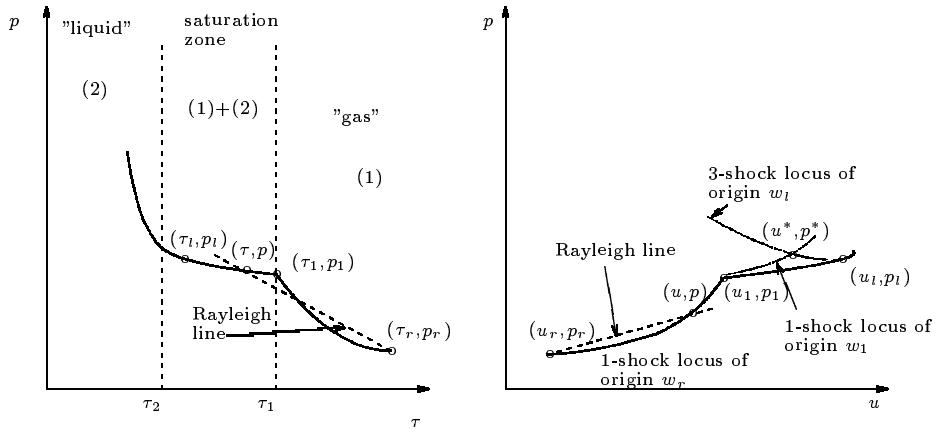

FIGURE 4.1. Non-uniqueness of the Riemann problem

Defining the Lagrangian velocity of the shock by

$$j = \rho_a(\sigma - u_a), \tag{4.5}$$

which does not depend on the side $(a) = (l)$ or $(a) = (r)$, we have equivalently

$$\begin{aligned} j^2 &= -\frac{[p]}{[\tau]}, \\ j &= \frac{[p]}{[u]}, \\ [\varepsilon] &+ \frac{1}{2}[\tau](p_l + p_r) = 0. \end{aligned} \tag{4.6}$$

If $j > 0$, we are in the case of a 3-shock, if $j < 0$, it is a 1-shock. The case $j = 0$ corresponds to a contact discontinuity. If V_r is fixed and if $j > 0$, equations (4.6) define a curve, called the Hugoniot curve, in the space (τ, u, p) of all the states V_l that can be connected to V_r by a 3-shock. This curve can parameterized by τ or j for instance (details can be found in [11], [13]).

4.2. **Non-uniqueness of the entropy solution .** We first construct an entropy solution made of a single shock wave. For this, we choose an arbitrary state $V_r = (\tau_r, 0, p_r)$ in the light phase, thus $\tau_r > \tau_1$. In the numerical experiments, we shall use, as in [13], $\tau_r = 1.3$ and $p_r = 0.1$. We choose also $\Gamma_1 = 0.6$ and $\Gamma_2 = 0.5$. This leads to $\tau_1 \simeq 1.092416506$ and $\tau_2 \simeq 0.9103470886$ (according to (3.19)).

We build the Hugoniot curve of origin V_r. As it it represented in figure 4.1, the projection of this curve on the plane (τ, p) is not convex at the point defined by $\tau = \tau_1$.

The left state V_l is chosen on the Hugoniot curve, inside the saturation region, thus $\tau_2 < \tau_l < \tau_1$. For the numerics, we take, as Jaouen [13], $\tau_l = 0.92$. Thanks to (4.6), the

pressure can be expressed as a function of τ along the Hugoniot curve

$$\left\{ \begin{array}{ll} p(\tau) = p_r \frac{(\Gamma_1+2)\tau_r - \Gamma_1 \tau}{\Gamma_1(\tau-\tau_r)+2\Gamma_1} & \text{if} \quad \tau_1 \leq \tau, \\ p(\tau) = p_r \frac{(\Gamma_1+2)\tau_r - \Gamma_1 \tau}{\Gamma_1(\tau-\tau_r)+2\tau_1} & \text{if} \quad \tau_2 \leq \tau \leq \tau_1. \end{array} \right. \tag{4.7}$$

Then, $p_l = p(\tau_l)$. The velocity u_l, the lagrangian velocity j_l, and thus the shock velocity σ along the Hugoniot curve are easily deduced from (4.6). This gives $u_l \simeq 0.1300665497$ and $p_l \simeq 0.1445192299$ and in this way, we have constructed one shock solution of the Riemann problem. It can be checked that it is entropic and satisfies the Lax characteristic condition. But this solution is not physical, i.e. has no viscous profile (details can be found in [13]).

It is indeed possible to construct another solution, which is the only physical solution. We keep the first part of the Hugoniot curve, outside the saturation region. The intersection of the Hugoniot curve and the plane $\tau = \tau_1$ provides us with a first state V_1 defined by $u_1 \simeq 0.08180962005$, $p_1 \simeq 0.1322415516$ and a shock velocity $\sigma_1 \simeq 0.5123360439$. Then, a Riemann problem is solved inside the saturation region

$$\begin{array}{l} W_t + F(W)_x = 0, \\ W(0,x) = \left\{ \begin{array}{ll} W_l & \text{if} \quad x < 0, \\ W_1 & \text{if} \quad x > 0. \end{array} \right. \end{array} \tag{4.8}$$

This Riemann problem has only one entropy solution, because inside the saturation region, the pressure law presents no pathology. Details are given in [13]. The physical solution has thus the form

$$V(t,x) = \left\{ \begin{array}{c} V_l \text{ if } x/t < \sigma_l, \\ V_{m,l} \text{ if } \sigma_l < x/t < u_m, \\ V_{m,1} \text{ if } u_m < x/t < \sigma_{m,1}, \\ V_1 \text{ if } \sigma_{m,1} < x/t < \sigma_1, \\ V_r \text{ if } \sigma_1 < x/t, \end{array} \right. \tag{4.9}$$

with

$$\begin{array}{l} V_{m,l} = (\tau_{m,l}, u_m, p_m), \\ V_{m,1} = (\tau_{m,1}, u_m, p_m). \end{array} \tag{4.10}$$

Just recall that, because only shock solutions occur, we have to find the intersection of the 1-shock locus of origin (u_1, p_1) and the 3-shock locus of origin (u_l, p_l). Thanks to (4.6), one has

$$\begin{array}{l} \tau_{m,l}(p_m) = \tau_l + 2\dfrac{p_l - p_m}{G(p_m + p_l)}, \\ \tau_{m,1}(p_m) = \tau_1 + 2\dfrac{p_1 - p_m}{G(p_m + p_1)}, \end{array} \tag{4.11}$$

$$\begin{array}{l} u_m = u_l - \sqrt{(p_m - p_l)(\tau_l - \tau_{m,l}(p_m)}, \\ u_m = u_1 + \sqrt{(p_m - p_1)(\tau_1 - \tau_{m,1}(p_m)}. \end{array} \tag{4.12}$$

Eliminating the intermediate velocity u_m from the equations of the two locus (4.12), we deduce the intermediate pressure $p_m \simeq 0.1450442653$. Then, one finds $u_m \simeq 0.1282046760$, $\tau_{m,l} \simeq 0.9133974480$, $\tau_{m,1} \simeq 0.9242879916$. The missing shock velocities are $\sigma_l \simeq -0.1293670530$ and $\sigma_{m,1} \simeq 0.3832619057$.

5. A simple finite volume scheme for the simulation of cavitating flows

In this section, we present numerical results in one dimension obtained with a new projection finite volume scheme. By projection (or relaxation) scheme we mean that each time step is made of two sub-steps. In the first sub-step a classical conservative scheme is employed. In the second sub-step, the projection (or relaxation) step, some variables are modified in order to stick to the equilibrium pressure law. This approach is very similar to the Boltzmann scheme approach (see [18] and included references).

We shall present three results.

The first result is obtained with the stiffened gas mixture model defined by the entropy (3.10). The phase transition is not taken into account and we observe the appearance of negative pressures or *tensions* in the liquid.

In the second test, we activate phase transition. We test the appearance of a bubble of vapor in a liquid subject to a strong drop of pressure. The pressure law coefficients that we use are based on physical measurements and are detailed in table 3.

In the third test, we try to compute the analytical solution constructed in section 4.2. We thus limit ourselves to a mixture of perfect gases whose entropy is given in (3.15).

For the conservative scheme in the first sub-step, we use the classical Godunov scheme. It is based on an exact Riemann solver for the problem:

$$v_t + f(v)_x = 0, \quad v(0,x) = \begin{cases} v_l \text{ if } x < 0, \\ v_r \text{ if } x > 0. \end{cases}$$

For the stiffened gas mixture, the conservative variables are $v = (\rho, \rho u, \rho\varepsilon + \rho\frac{u^2}{2}, \rho\alpha, \rho y)^T$, the flux is $f(v) = (\rho u, \rho u^2 + p, (\rho\varepsilon + \rho\frac{u^2}{2} + p)u, \rho\alpha u, \rho y u)^T$. The pressure law is given by (3.4-3.9).

For the perfect gas model, the volume fraction α and the corresponding part of the flux are useless, because we have already supposed the pressure equilibrium.

We denote by $R(v_l, v_r, \frac{x}{t})$ the self-similar solution v. As proven in [19], the Riemann problem has a unique global entropic solution.

Let h be a space step and τ a time step. Let $x_i = ih$, $t_n = n\tau$ and $w_i^n \simeq w(t_n, x_i)$ where w is an entropic solution of $w_t + f(w)_x = 0$. The classical Godunov step is

$$\frac{w_i^{n+1/2} - w_i^n}{\tau} + \frac{F_{i+1/2}^n - F_{i-1/2}^n}{h} = 0.$$

This first step provides us with a density $\rho^{n+1} = \rho^{n+1/2}$, a velocity $u^{n+1} = u^{n+1/2}$ and an internal energy $\varepsilon^{n+1} = \varepsilon^{n+1/2}$. The volume fraction $\alpha^{n+1/2}$ and the mass fraction $y^{n+1/2}$

have to be updated (projected) to take into account phase transition. Physically, the stable state corresponds to a maximum of the specific entropy, we thus define (α^{n+1}, y^{n+1}) by

$$s(1/\rho^{n+1}, \varepsilon^{n+1}, \alpha^{n+1}, y^{n+1}) = \max_{(\alpha,y)\in[0,1]\times[0,1]} s(1/\rho^{n+1}, \varepsilon^{n+1}, \alpha, y).$$

For the perfect gas model the volume fraction is not present and we optimize only with respect to the mass fraction y.

5.1. **Numerical scheme for the metastable case.** In order to illustrate our approach, we first recall what happens if the cavitation is not taken into account. The test case is a Riemann problem which presents two rarefaction waves in water. It is intended to demonstrate the apparition of negative pressures when cavitation is not taken into account ([9], [4]).

The simulation time is of 0.2 ms, the discretization is of 1000 cells. The length of the study interval is 1 m. The initial data are given in the table 1, and the numerical parameter for the stiffened gas law are given in the table 3. The numerical results are on figures 5.1, 5.2, 5.3. We observe two rarefaction waves moving in the opposite directions.

	Left state	Right state
ρ	1000 kg/m^3	1000 kg/m^3
u	-100 m/s	100 m/s
p	1×10^5 Pa	1×10^5 Pa

TABLE 1. *Initial data for the Riemann problem*

5.2. **Numerical scheme for the transition case.** In this part, the second sub-step (optimization of the entropy) is activated. On the same test case as above, we obtained the results of figures 5.4, 5.5, 5.6, 5.7, 5.8.

We observe a vapor bubble in the center of the computation domain and the pressure remains positive. This is only a qualitative validation.

5.3. **Comparison with the analytical solution.** In this section, we present the numerical results obtained with the projection scheme for the analytical solution presented in section 4.2. Numerical results are given in figures 5.9, 5.10, 5.11. We observe an excellent agreement between the numerical and the exact solution. The presented results have been obtained with a CFL number of exactly one. There is no oscillation and the viscous solution is well captured. We have also performed tests for lower CFL numbers and captured exactly the same solution. Other one-dimensional tests can be found in [3]. Let us recall that classical Godunov schemes can converge to various entropy solutions according to the CFL number as observed by Jaouen in [13].

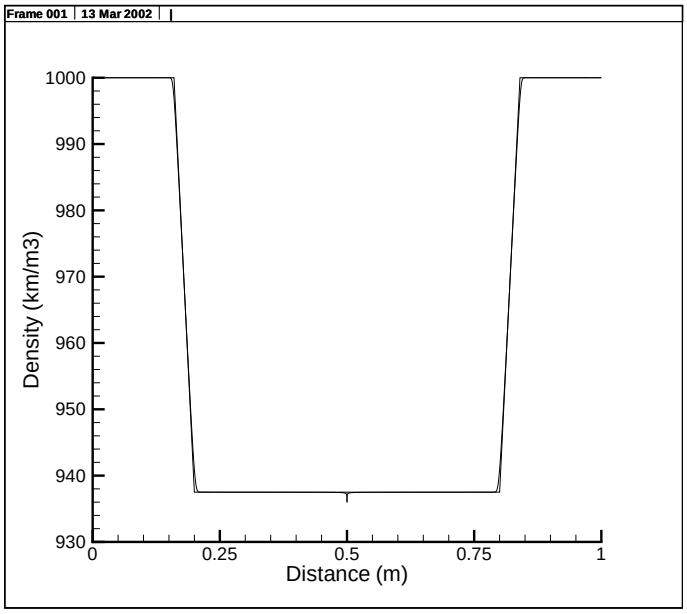

FIGURE 5.1. *Density in the metastable case*

6. The hypersonic underwater projectile

In this section, we present a more physical simulation. It consists in a hypersonic two-dimensional projectile dived into still water at a velocity of 1000 m/s. In the wake of the projectile appears a vapor cavitation pocket. This test has been studied by Butler, Cocchi and Saurel in [21].

6.1. **Tuning of the temperature law.** We have first to compute adequate pressure law coefficients in order to obtain realistic results. In order to fix the constants, we have tried to respect some physical realities such as saturation curve, specific heat, sound speed.

At temperature $T = 372.76K$, the known physical values are reproduced in the table 2 and are extracted from the book of Lide [16]:

	Vapor	Water
Enthalpy : h (J.g^{-1})	2674.9×10^3	417500
γ	1.3	3.
C_p (J.kg^{-1}.K^{-1})	2100	4200

TABLE 2. *Experimental values for the setting of the temperature law*

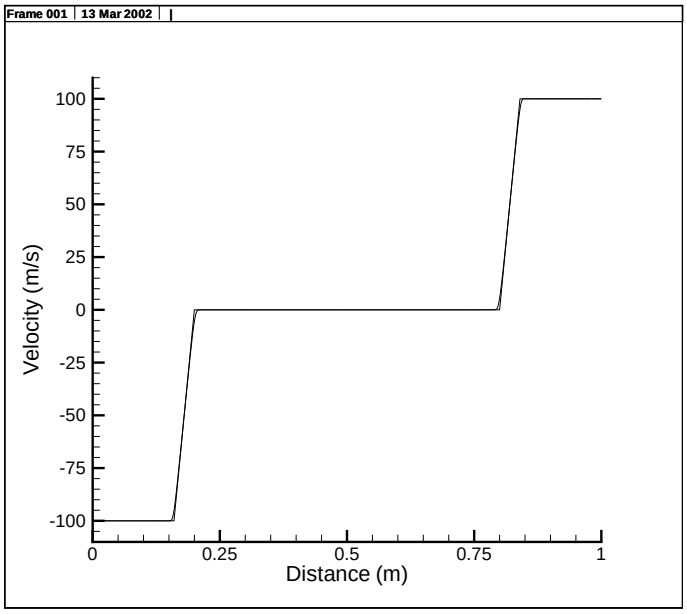

FIGURE 5.2. *Velocity in the metastable case*

Thanks to the relation :

$$h = Q + C_p T, \tag{6.1}$$

where h is the enthalpy, Q the energy of formation and C_p the specific heat at constant pressure, we are able to compute the values of Q_1 and Q_2 :

$$Q_1 = 0.1892 \times 10^7 \mathrm{J/kg} \tag{6.2}$$

$$Q_2 = -0.1148 \times 10^7 \mathrm{J/kg} \tag{6.3}$$

The computation of the pressure constant π_2 for the liquid water is based on the sound speed in water. The sound speed in water, c, is approximately 1600 m.s^{-1} at ambient pressure and temperature. Then, thanks to the relation:

$$\pi_2 = \frac{\rho_0 c^2}{\gamma_2}, \tag{6.4}$$

where $\rho_0 = 1000$ kg.m^{-3} is the density of water at ambient pressure and temperature, we obtain $\pi_2 = 8533 \times 10^5$ Pa. In vapor, $\pi_1 = 0$ Pa.
In order to compute the constant K appearing in (3.15), we use the values of the specific

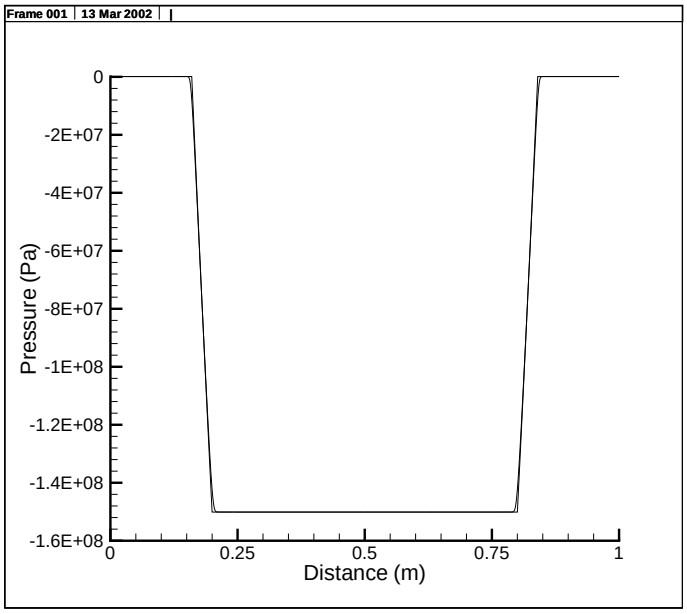

FIGURE 5.3. *Pressure in the metastable case*

heats at constant volume given in [16]:

$$C_{v,1} = \frac{C_{p,1}}{\gamma_1} = 1615.38 \text{ J.kg}^{-1}.\text{K}^{-1} \tag{6.5}$$

$$C_{v,2} = \frac{C_{p,2}}{\gamma_2} = 1400 \text{ J.kg}^{-1}.\text{K}^{-1} \tag{6.6}$$

Finally, the constant K is obtained by:

$$K = (C_{v,1} - C_{v,2}) \ln(T_0) + \tag{6.7}$$

$$\frac{(Q_2 - Q_1)}{T_0} + (\gamma_1 - 1) C_{v,1} \ln\left(\frac{(\gamma_1 - 1) C_{v,1} T_0}{(p_0 + \pi_1)}\right) - (\gamma_2 - 1) C_{v,2} \ln\left(\frac{(\gamma_2 - 1) C_{v,2} T_0}{(p_0 + \pi_2)}\right), \tag{6.8}$$

The ambient pressure is $p_0 = 10^5 Pa$ and the ambient temperature $T_0 = 273.76K$.

The physical constants of the stiffened gases model are summed up in 3.

6.2. **Numerical results.** In this part, we present the numerical results in 2D. The projectile and the computation domain are described in the graphic 6.1. The horizontal velocity of the projectile is -1000 m.s^{-1}, it is thus moving from the right to the left. By a change of

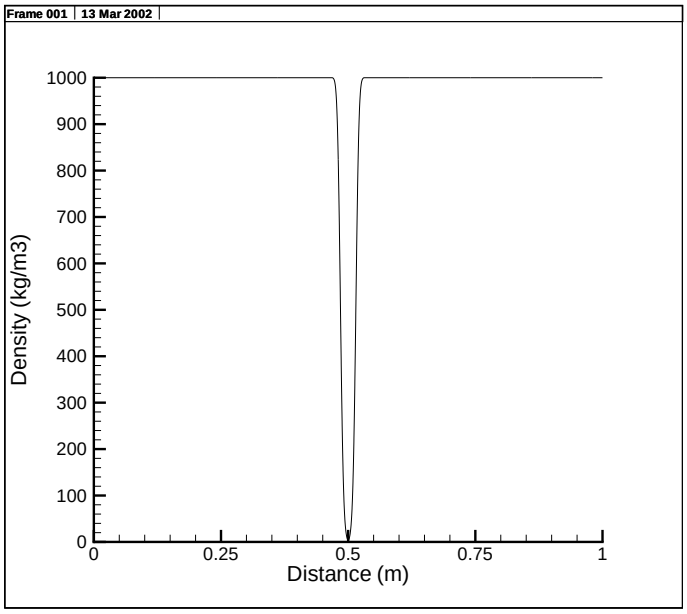

FIGURE 5.4. *Density in the transition case*

	fluid 1 (vapor)	fluid 2 (water)
γ	1.3	3
π	0	8533 bar
Q	0.1892×10^7 J/kg	-0.1148×10^7J/kg
C_v	1615.38 J/kg/K	1400 J/kg/K

TABLE 3. *Constants in the stiffened gas model*

referential, we can also suppose that the projectile is fixed and impose a velocity of water of 1000 m.s^{-1}.
On the boundary of the projectile, the upper and the downer parts of the domain boundary, we impose a mirror condition. On the inner and outer parts of the boundary, we impose the nature of the flow: $\rho = 1000$ kg.m^{-3}, $p = 10^5$ Pa, horizontal velocity $u = 1000$ m.s^{-1}, vertical velocity $v = 0$. We take the same values for the initial condition in the domain in order to model the sudden arrival of the projectile in water.

Density, pressure, velocity modulus and volume fraction of water are represented at time $t = 225$ms on figures 6.2, 6.3, 6.4 and 6.5.

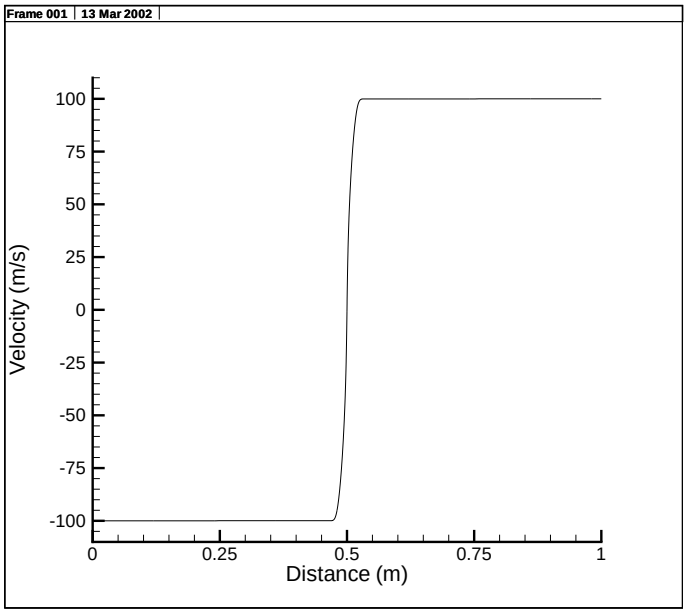

FIGURE 5.5. *Velocity in the transition case*

7. CONCLUSION

In this paper, we have first constructed a model for liquid-vapor phase transition. Returning to thermodynamics we have shown how to properly construct pressure laws for a mixture of two fluids. It appears that the equilibrium pressure law corresponds to a maximum of the mixture entropy with respect to the volume, mass and energy fractions of the vapor. using this representation, it was possible to propose a new projection finite volumes scheme for the numerical simulation of cavitation. Each time step of this scheme is made of two stages. In a first stage, the flow is solved by a classical Godunov scheme, with exact Riemann solver, without taking into account phase transition. This is possible because the mixture pressure law is simpler than the equilibrium pressure law. In a second stage, the fractions are updated in order to recover the equilibrium pressure law by a maximization of the mixture entropy. This scheme has been tested first on an analytical solution. It was able to recover the unique physical solution (the viscous solution) even if several entropy solutions are possible. Finally, we illustrated the ability of the scheme to deal with more physical configurations in 2D.

Now this work could be extended in several directions:

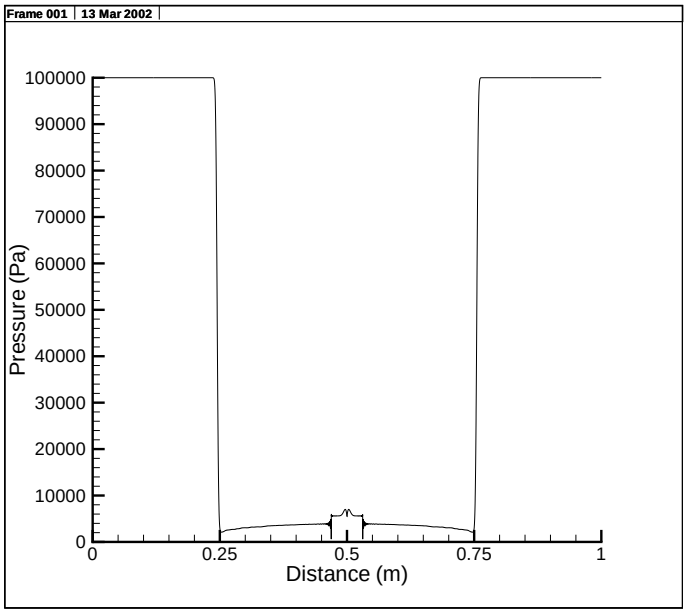

FIGURE 5.6. *Pressure in the transition case*

(1) First of all, it would be interesting to improve the precision of the mixture law. Indeed, in its present form, the model is not able to take into account the critical point. The critical point is a special point of the phase diagram in the temperature-pressure plane. It corresponds to the upper extremity of the saturation curve. Beyond this point there is no more distinction between the two phases. We expect that this behavior can be modelled by only changing the entropy function of the liquid phase.

(2) Another interesting extension would be to add a supplementary inert phase in order to simulate, for instance, air-water flows, with the possibility to observe a cavitation phenomenon in water. The model is a simple extension of what is done in part 2.3. The mixture entropy is the sum of the three phases entropies (as in formula 2.25) and depends on density, internal energy, air fractions and vapor fractions. In the optimization process, we maximize the mixture entropy with respect to all the fractions excluding the mass fraction of air, because there is no mass transfer between air and water. The mass fraction of air is thus simply convected. Despite its simplicity this approach leads to numerical difficulties. According to our first experiments, numerical pressure oscillations appear at the interface between air and water [3]. These oscillations are similar to those observed in many works about two-phase flows [1], [14], [20]... It is interesting to observe that the maximization of entropy insures stability of the numerical scheme. If one forgets to optimize with respect to one variable, it can be sufficient to imply oscillations.

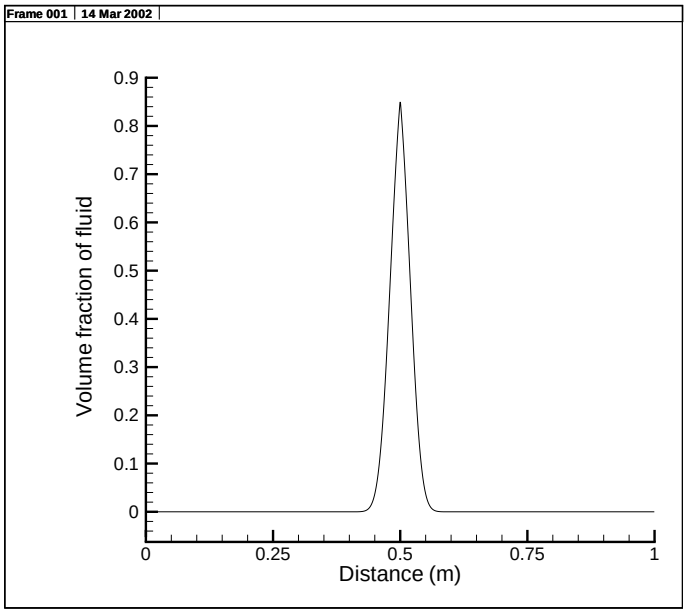

FIGURE 5.7. *Vapor volume fraction in the transition case*

(3) Finally, it appears that the equilibrium hypothesis is physically not true for very fast flows. It is even possible to observe during a short time negative pressures in the liquid before the phase transition [9]. It is clear that one should then give a finite value to the parameter λ in the source term (2.16). This value is linked to the time scale of the phase transition. Instead of solving numerically an ordinary differential equation one could imagine for instance to perform only a partial optimization of the mixture entropy.

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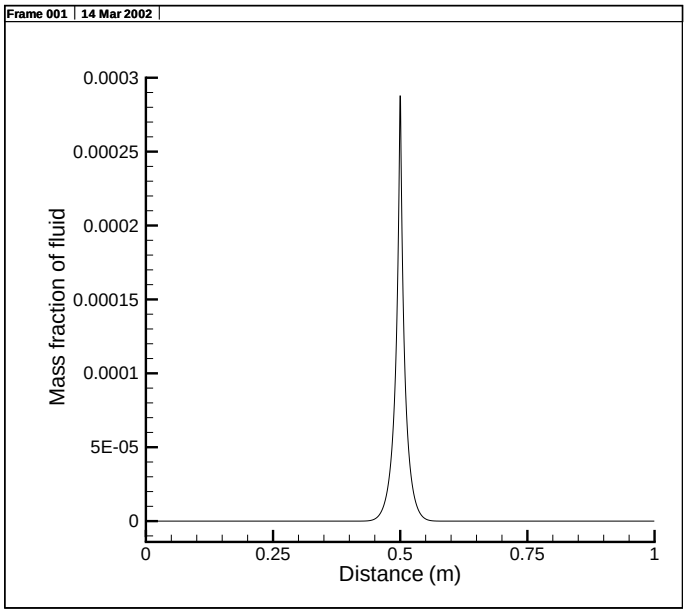

FIGURE 5.8. *Vapor mass fraction in the transition case*

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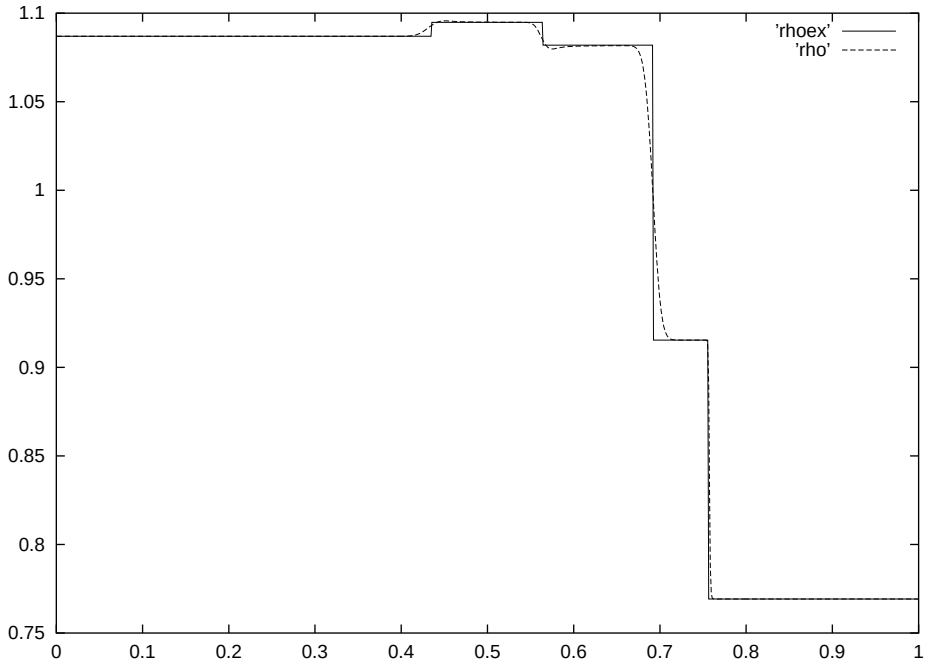

FIGURE 5.9. *Numerical and exact density for the relaxation scheme*

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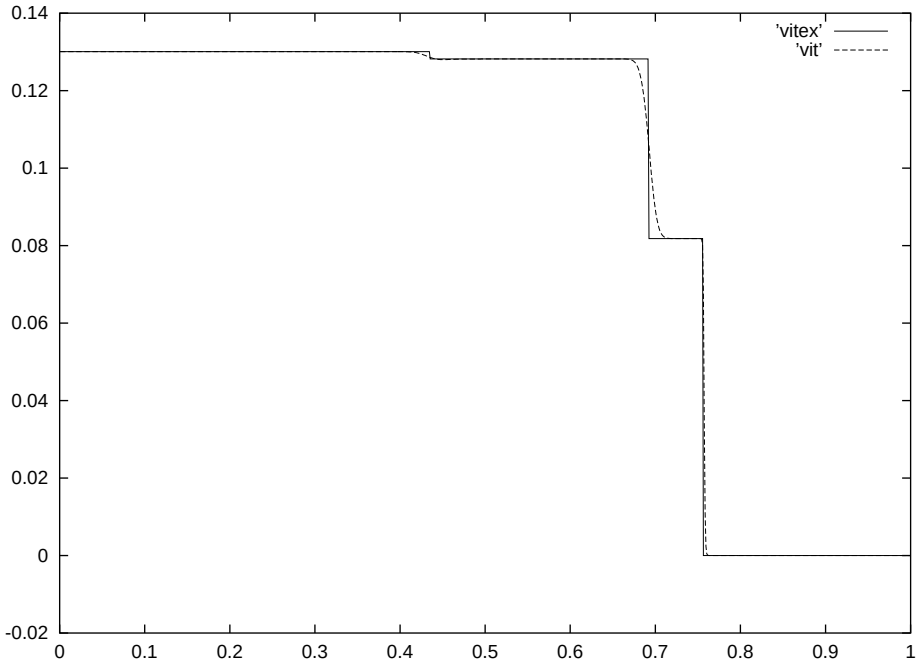

FIGURE 5.10. *Numerical and exact velocity for the relaxation scheme*

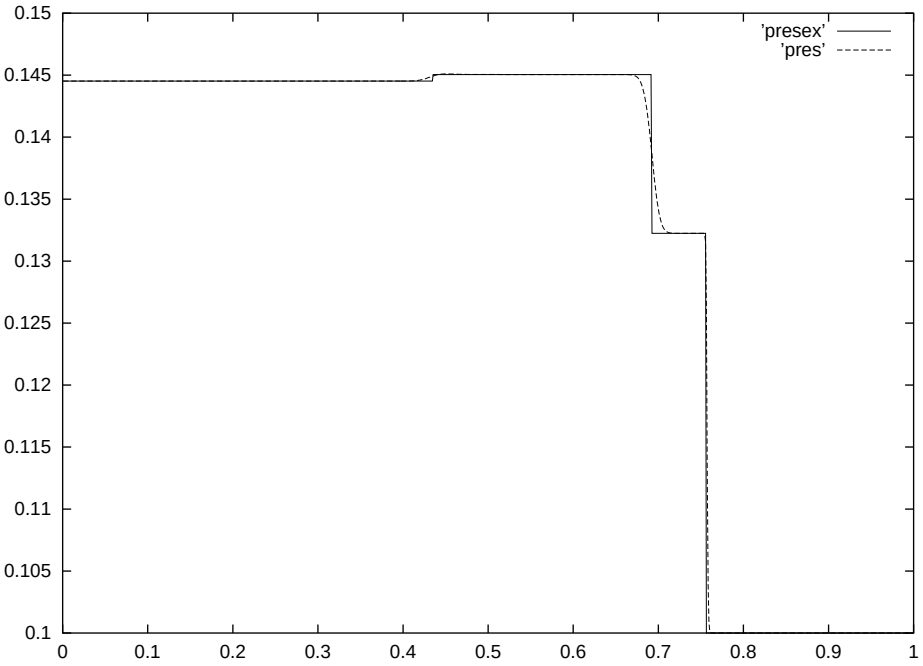

FIGURE 5.11. *Numerical and exact pressure for the relaxation scheme*

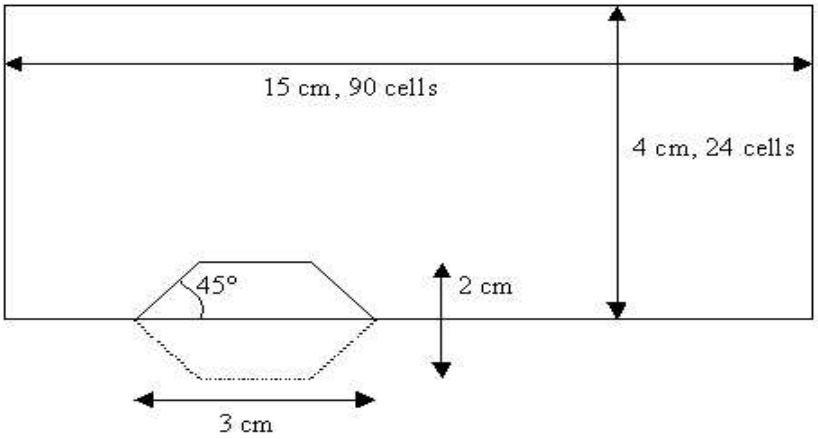

FIGURE 6.1. *Geometry description*

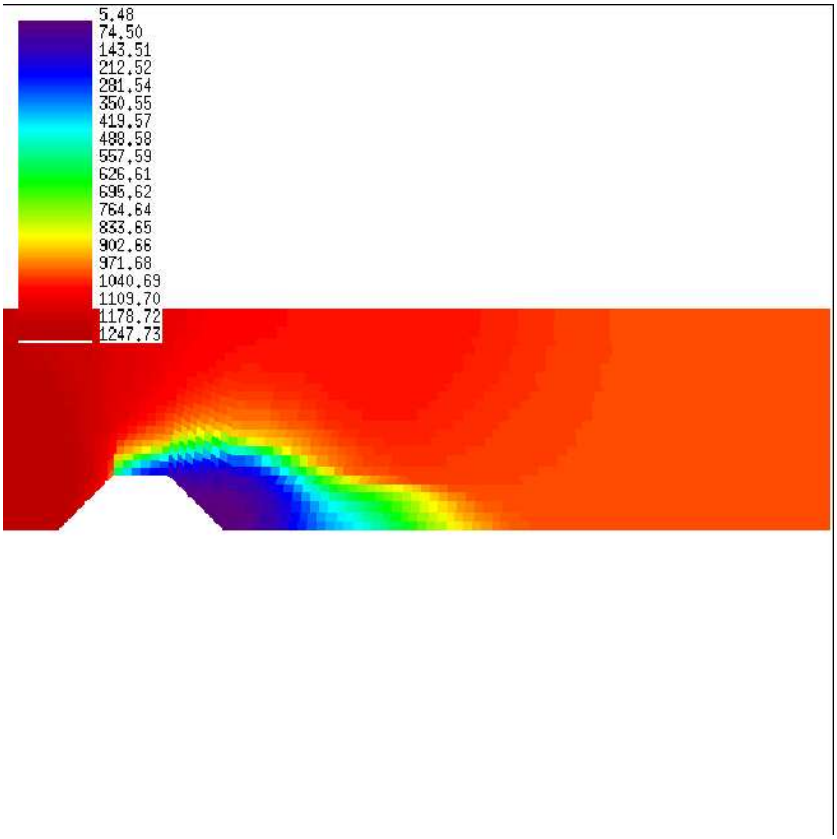

FIGURE 6.2. *Density at 225 ns*

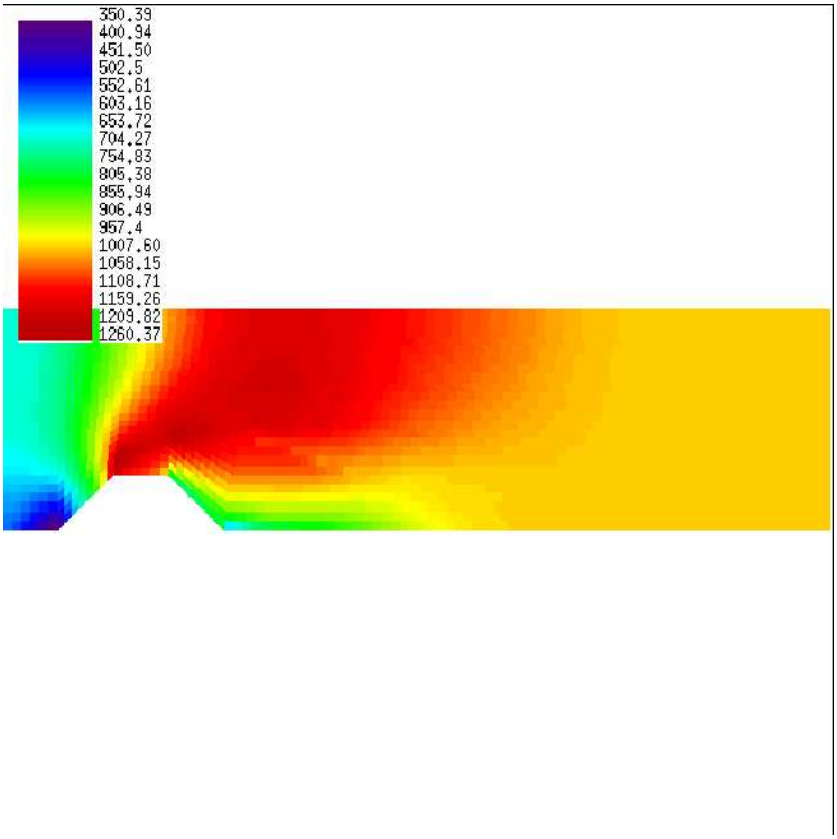

FIGURE 6.3. *Velocity modulus at 225 ns*

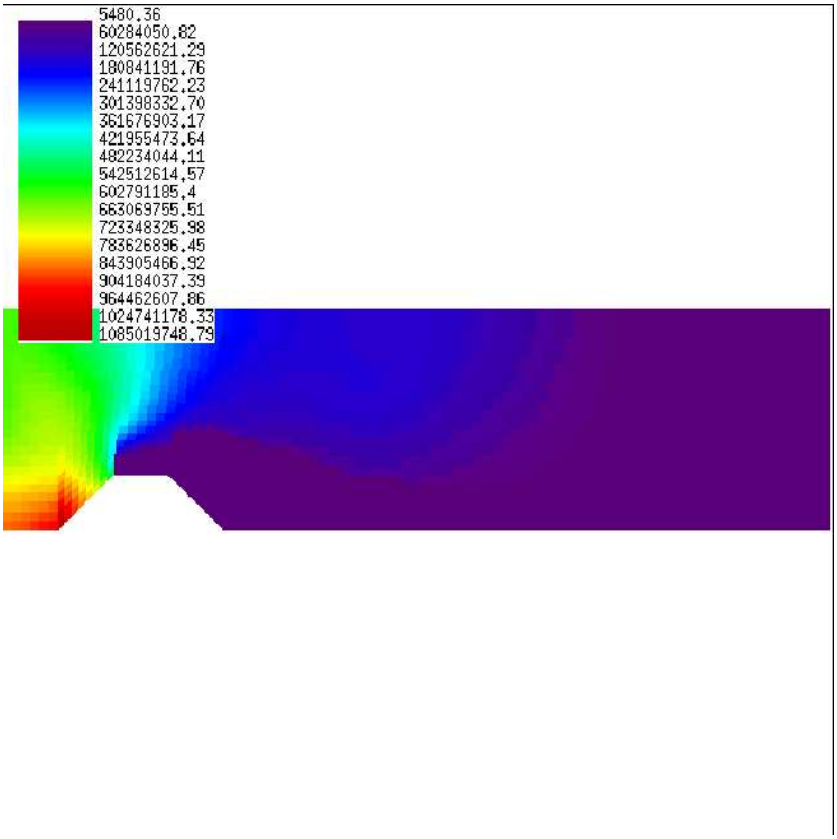

FIGURE 6.4. *Pressure at 225 ns*

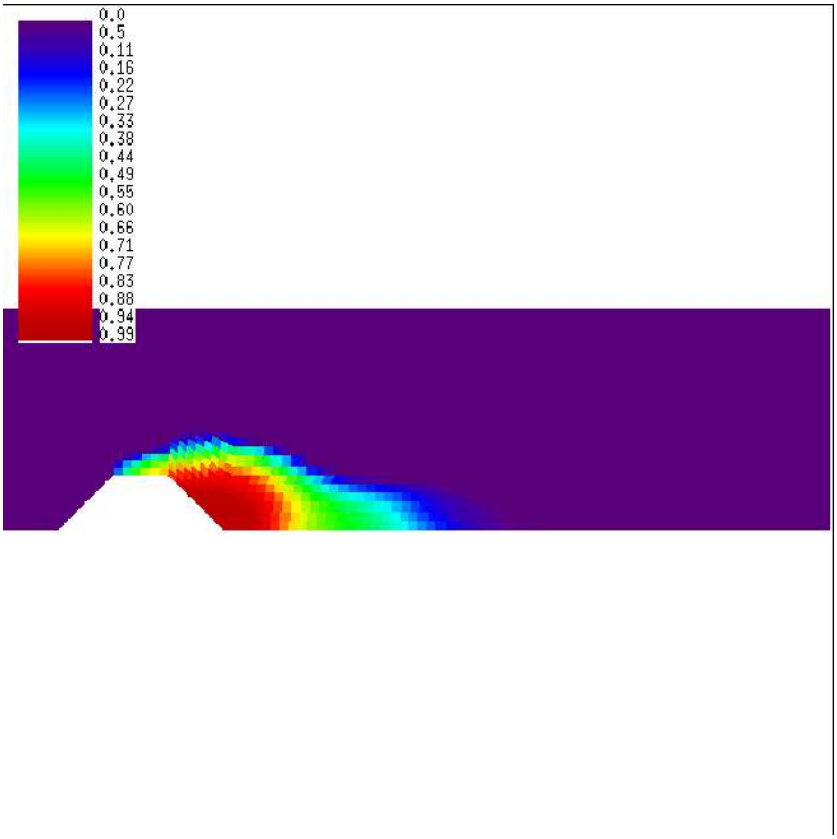

FIGURE 6.5. *Vapor volume fraction at 225 ns*

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